

1,5-Dimethyl-6-phenyl-1,6-dihydro-3-pyridinecarbonitrile
27531-49-3 | DTXSID30297547

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.78

Global applicability domain: Inside

Local applicability domain index: 5.76e-01

Confidence level: 7.53e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1-Piperidineacetamide, N-(2-bromophenyl)-

Measured: 2.94

Predicted: 3.12

[Image not found](#)

1-Piperidineacetamide, N-(3-chlorophenyl)-

Measured: 3.45

Predicted: 3.22